Phenol, 2-[1-(4-hydroxyphenyl)-1-methylethyl]-837-08-1 | DTXSID7042275

037-00-1 D17/31D7/042273

Model Performance

Model	Data

Weighted KNN model

5-fold CV (5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.87	0.81	0.87	0.82	0.86	0.86	

Model Results

Predicted value: 2.75e-03 mol/L

Global applicability domain: Inside

Local applicability domain index: 3.65e-01

Confidence level: 5.72e-01

Nearest Neighbors from the Training Set

Image not found

1,3-Naphthalenediol Measured: 1.12e-02 Predicted: 2.01e-02

Image not found

1,5-Dihydroxynaphthalene Measured: 1.03e-03 Predicted: 8.87e-03